# DF 4: Glasses (Joint Session with DY and CPP)

Time: Monday 15:00–17:30 Location: ZEU 146

DF 4.1 Mon 15:00 ZEU 146

**Dynamic Crossover and Stepwise Solidification of Confined Water** — •Matthias Sattig and Michael Vogel — Hochschulstraße 6, D-64289 Darmstadt

The dynamical behaviour of water in the regime of the supercooled liquid is still a topic of large interest. In particular, the existence of a fragile-to-strong transition (FST) at around 225K induced by a liquid-liquid phase transition (LL) is controversially discussed [1]. The proposed temperature range of the FST is hardly accessible in bulk water.

Our $^2$H NMR investigation reveals two dynamic crossovers of supercooled water in nanoscopic (nm) confinement. A dynamic crossover of liquid water at ca. 225K is accompanied by a formation of a fraction of solid water. Therefore, this effect can not be attributed to the LL, but rather to a change from liquid-like to interface-dominated dynamics. Moreover, the $^2$H NMR data yield evidence that the $\alpha$ process and $\beta$ process are observed in experiments above and below this temperature, respectively. Upon cooling through a dynamic crossover at ca. 175K, the dynamics of the liquid fraction becomes anisotropic and localized, implying solidification of the corresponding water network, most probably, during a confinement-affected glass transition.

[1] Mishima; Nature, Vol. 396, 329(1998)

DF 4.2 Mon 15:15 ZEU 146

**Understanding the nonlinear mobility of single driven particles in supercooled liquids** — •Carsten F. E. Schroer[1,2] and Andreas Heuer[1,2] — [1]WWU Münster, Münster, Germany — [2]Graduate School of Chemistry, Münster, Germany

We perform MD simulations of a binary Lennard-Jones mixture where a single particle is pulled by an external field through the liquid. Herein, we are specifically interested in the range of intermediate and strong forces when nonlinear effects occur in the single particle dynamics.

It is known from experimental and simulation studies, that the steady-state velocity $\overline{v}$ follows in the limit of low forces a linear response relation $\overline{v} = \mu F$ where the force $F$ is connected to the dynamical response via the constant mobility $\mu_0 = \frac{D_0}{k_B T}$. For large forces, however, one finds a dramatic increase of $\overline{v}$ with increasing $F$, indicating a nonlinear force-dependence of the mobility, i.e. $\mu_0 \to \mu(F)$.

To gain a deeper understanding of this behavior, we studied the underlying potential energy landscape of the system by computing the minima the system has resided in during its time-evolution. This immediately allows us to discuss the nonlinear mobility in terms of thermodynamical (distribution of energies) and kinetic (escape rates out of single minima) quantities. Most interestingly it turns out, that both effects are of major importance for the nonlinearity of the system, so that there is no single nonlinear effect but an interplay of two independent which contributes to the dynamical responses of the driven particles.

DF 4.3 Mon 15:30 ZEU 146

**Simulation of Borate glasses** — •Christoph Scherer[1,2], Friederike Schmid[1], Martin Letz[2], and Jürgen Horbach[3] — [1]Johannes Gutenberg-Universität, Mainz — [2]Schott AG, Mainz — [3]Heinrich-Heine-Universität, Düsseldorf

The model glass former B2O3 is studied as an example for generating accurate glass structures on the computer. B2O3 is an important component for the simulation of oxide glasses since boron can form triangular planar structures, as well as tetrahedral nearest neighbor structures and also boroxol rings. In one approach, configurations of a few hundred atoms are equilibrated at high temperature, well above the glass transition temperature, with a classical molecular dynamics simulation (MD). After a quench down to 0K, they are structurally relaxed by means of an ab inito (DFT) calculation. The structural and vibrational properties are compared to the results of a full ab inito quench to 0K and to experimental results. The dependence of the glass structure and the liquid properties on the classical force field is examined. Therefore, a set of classical force fields is generated by means of a structural fitting procedure. The parameters are fitted in a way that the structure, namely the radial distribution functions and the angular distributions, of a classical MD run matches as closely as possible the structure of an ab initio (DFT) run at the same temperature. Parameter fits are carried out according to an ab initio trajectory at high temperature, where the system is in the liquid state. This sets the basis for the next steps: The development of a classical force field for sodium-borate glasses by the same methodology.

DF 4.4 Mon 15:45 ZEU 146

**Mixing random organization and jamming** — •Michael Schmiedeberg — Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany

The random organization and the athermal jamming transition can both be studied in a unifying model system. We study the mixture of the protocols of the two transitions and argue that such a mixture can be interpreted as the glass transition at small but non-zero temperatures.

In our model system, first particles are randomly distributed and then in each step overlapping particles are displaced. In case of displacements in random directions the so-called random organization transition is observed. For purely deterministic displacements the jamming transition is realized. While the jamming protocol match with a quench of a soft sphere system from infinite to zero temperature without crossing energy barriers, the random displacements of the random organization protocol correspond to thermally activated rearrangements of particles. If in a mixed protocol the probability of random displacements is small but non-zero we find that the transition differs significantly from the purely deterministic jamming transition. We believe that our model system can help to understand why there is a difference between the glass transition at small but non-zero temperatures and the athermal jamming transition.

DF 4.5 Mon 16:00 ZEU 146

**Existence of glass-form factors** — •Thomas Franosch — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, A-6020 Innsbruck, Austria

A hallmark of the glass transition is the slow structural relaxation of a quasi-arrested structure. As an idealization the dynamics is considered to become non-ergodic directly at the glass transition such that all auto-correlation function coupling to the structural relaxation exhibit finite non-trivial long-time limits often referred to as glass-form factors or nonergodicity parameters. Simultaneously, the theory of stochastic processes in the framework of probability theory imposes quite stringent conditions on the class of correlation functions. The existence of a finite limit at long times is then connected to the properties of the associated spectral measure, and in general correlation functions can either oscillate forever, display quasi-periodic behavior, or even intermittent behavior. While for purely relaxation dynamics, e.g. Brownian dynamics, the existence of a long-time limit is trivial, the situation for the case of Newtonian dynamics has been elusive so far.

In this talk I elaborate conditions covering a broad class of theoretical approaches that guarantee the existence of a long-time limit. As a special case I show that the mode-coupling theory of the glass transition belongs to that class. As an outlook I briefly discuss the case of multiple decay channels relevant for molecular or confined systems.

**15 min break**

DF 4.6 Mon 16:30 ZEU 146

**Spin freezing in geometrically frustrated magnets** — Jorge Rehn[1], Arnab Sen[1,2], •Alexei Andreanov[1], Antonello Scardicchio[3], Kedar Damle[4], and Roderick Moessner[1] — [1]Max-Planck Institut fur Physik komplexer Systeme, Dresden, Germany — [2]Indian Association for the Cultivation of Science, Kolkata, India — [3]The Abdus Salam ICTP, Trieste, Italy — [4]The Tata Institute, Mumbai, India

Materials which are believed to be faithfully represented by classical frustrated magnets with macroscopically degenerate groundstates, often exhibit spin-freezing. The latter is a transition to a spin-glass phase. Explaining the mechanism of such freezing is not always a simple task, since conventional ingredients, like randomness of the interactions, is not always present in the systems under study. We present a model, where dilution alone generates frustrating interaction between certain spins in the systems and leads to their freezing. The effective

model deals with antiferromagnetically coupled Heisenberg spins in 2D. Both the long-range nature of the interaction and its dependence on the distance are crucial for the existence of the glass phase. We confirm our predictions by performing Monte-Carlo simulation of the effective model.

DF 4.7 Mon 16:45 ZEU 146

**Glasses of binary colloidal mixtures in the quiescent state and under shear** — •Tatjana Sentjabrskaja, Marco Laurati, and Stefan Egelhaaf — Condensed Matter Physics Laboratory, Heinrich-Heine Universität Düsseldorf, D-40225 Düsseldorf, Germany

We investigate mixing effects on the glass state of binary colloidal hard sphere mixtures with large size asymmetry (size ratio 1:5). Increasing the amount of small spheres in a system of large ones, a glass-glass transition is observed, where the large particles, initially caged by the large spheres, become localised in a cage of small spheres [1]. During the transition, the dynamics accelerate and a strong reduction of the yield strain as a result of the shift of random close packing is observed[2].

The results of rheology are compared to measurements of the dynamics of particles under shear. The super-diffusion typically associated with stress overshoots [3] becomes more pronounced for mixtures in which the dynamics are increasingly arrested. Moreover, we observe different degrees of shear-induced constriction depending on mixing ratio, which closely follow changes in the magnitude of the stress overshoot.

[1] T.Sentjabrskaja et al., AIP Conf.Proc., 1518, 206, 2013.
[2] T.Sentjabrskaja et al., Soft Matter, 9(17), 4524- 4533, 2013.
[3] M.Laurati et al., J. Phys.: Condens. Matter, 24, 464104, 2012.

DF 4.8 Mon 17:00 ZEU 146

**Microscopic theory for sheared colloidal glasses and gels** — •Christian Amann and Matthias Fuchs — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

We use mode coupling theory (MCT) to calculate in three dimensions (3D) transient density autocorrelators in start-up shear flow. It is thus possible to quantitatively predict flow curves and distorted structure of colloidal glasses and gels under shear flow. We investigate the transient, non-linear, non-monotonous stress response to strain and structure-factor distortion in 3D as well as steady-state flow curves (cf. [1] for 2D calculations). Density correlators, stress response, and structure-factor distortions are in good qualitative agreement with experiments [2], while the quantitative errors of the theory can be identified. A close connection between the time-evolution of symmetries of structure-factor distortions and non-monotonous stress response (i.e. stress overshoot) can be observed. We use as input a structure factor calculated with analytical Percus Yevick closure, which allows to approximate a hard sphere repulsion as well as augmenting a short range square-well attraction [3]. Hence, implications of a gel-glass to repulsive-glass transition on the transient rheology can be studied.

[1] Amann, C.P. et al. *J. Rheol.* **57**, 149 (2013); Henrich O. et al. *Phil. Trans. R. Soc. A* **367**, 5033 (2009)
[2] Denisov, D. et al. *Sci. Rep.* **3**, 1631 (2013)
[3] Dawson K. et al. *PRE* **63**, 011401 (2000)

DF 4.9 Mon 17:15 ZEU 146

**An efficient Monte Carlo algorithm to study structural relaxation in network forming materials** — •Richard Vink — Institute of Theoretical Physics, Georg-August-Universität Göttingen, Germany

Network forming materials are ubiquitous in nature, common examples being semiconductors such as silicon and silica, as well as fluids that can form hydrogen bonds. What these materials have in common is that their topology on short length scales is governed by certain rules. For example, in amorphous silicon, most atoms are 4-fold coordinated, the preferred Si-Si bond length being $\approx$ 2.35 Å, and the preferred Si-Si-Si bond angle being the tetrahedral angle. This complicates molecular dynamics simulations of these materials, where the particles spend most of their time thermally fluctuating about their equilibrium positions, while large structural changes in the network topology are rare. To overcome this problem, Wooten, Winer, and Weaire (WWW) introduced a special Monte Carlo move consisting of bond switching Monte Carlo moves which turned out to be very efficient at structurally relaxing networks of amorphous silicon and silica [Phys. Rev. Lett. **54** 1392 (1985)]. Unfortunately, the algorithm is only correct when used at zero temperature. In order to also address finite temperature, I propose a modification to the original WWW algorithm such that the Boltzmann distribution is faithfully sampled at any given temperature. The resulting algorithm is used to study the melting transition of a two-dimensional three-fold coordinated network.